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WATER TREATMENT MODEL FOR POLLUTANT EXPOSURE ASSESSMENT: SYSTEM DOCUMENTATION AND USERS MANUAL

by

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FOREWORD

Environmental protection efforts are increasingly directed towards preventing adverse health and ecological effects associated with specific compounds of natural or human origin. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Technology Development and Applications Branch develops and evaluates management or engineering tools for assessing and controlling adverse environmental effects of these substances.

Solutions to serious environmental pollution problems increasingly involve analyzing and evaluating difficult trade-offs between useful substances and products and the risk posed to human health and environmental quality from toxic materials. One method for estimating the actual human and environmental exposure to substances and their effects is the application of mathematical models. This report describes the development and use of a mathematical exposure assessment model of some potable water treatment processes. It is envisioned that this model will be linked to other models for use as part of exposure assessments.

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ABSTRACT

A mathematical model of potable water treatment to remove toxic substances has been developed for use in exposure assessment modeling. Treatment processes modeled include sedimentation, coagulation-flocculation, filtration, aeration, chemical oxidation, and granular activated carbon adsorption. Besides describing the use of the program, this users manual presents example runs of the model.

This report covers the period January 1979 to November 1982, and work was completed as of August 1983.

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LIST OF ABBREVIATIONS AND SYMBOLS

ABBREVIATIONS

A -- external mass transfer area (m^2)
AB -- biofilm surface area per carbon particle (m^2)
AP -- atmospheric pressure (torr)
C -- aqueous concentration of substance (mg/l)
CD -- coefficient of discharge (dimensionless)
Conc -- concentration of chemical ($mole^{-1}$)
CP -- partition coefficient (dimensionless)
DB -- diffusivity of solute in biomass ($m^2\ hr^{-1}$)
DCP -- diameter of carbon particle (m^2)
DL -- free liquid diffusivity of solute ($m^2\ hr^{-1}$)
DTF -- detention time for the flocculation basin (min)
DTS -- detention time for sedimentation basin (hrs)
E -- packed bed porosity (dimensionless)
eff -- effluent (subscript)
EPEX -- expanded bed porosity (dimensionless)
F -- fraction of toxicant associated with particulate matter (dimensionless)
G -- gravitational constant ($ft\ sec^{-2}$)
h -- head on nozzle (ft)
inf -- influent (subscript)
JD -- mass transfer factor (dimensionless)
K -- rate constant (T^{-1})
K2 -- 2nd order chemical oxidation rate constant at pH 7 and 20°C ($l\ mole^{-1}\ hr^{-1}$)
KF -- hydrodynamic film mass transfer coefficient ($m\ hr^{-1}$)
KOX -- removal rate constant for chemical oxidation (hr^{-1})
KPD -- removal rate constant for photodegradation (hr^{-1})
KV -- removal rate constant for volatilization (hr^{-1})
MV -- viscosity of water ($mg\ m^{-1}\ hr^{-1}$)
MW -- molecular weight of compound to be removed
NCPC -- number of carbon particles present
NRE -- Reynolds number
NSC -- Schmidt number
O_2 -- oxygen solubility ($mg\ l^{-1}$)
OF -- overflow rate ($gpd\ ft^2$)
Q -- flowrate (MGD)
QE -- fixed phase concentration (dimensionless)
rem -- removed (subscript)
RHOBC -- combined density of carbon and biomass ($mg\ m^{-3}$)
RHOCP -- mass of carbon per unit carbon volume ($mg\ m^{-3}$)
RHOL -- density of solvent ($mg\ m^{-3}$)
RHOPAC -- mass of carbon per unit contactor volume ($mg\ m^{-3}$)

RXC -- removal rate by adsorption (mg m^{-3} hr^{-1})
RXS -- removal rate by bio-oxidation (mg m^{-3} hr^{-1})
S -- liquid concentration (ML^{-3})
S* -- concentration within carbon averaged over entire carbon particle (mg l^{-1})
SA -- surface area of filter (100 ft^2)
Sed -- sediment concentration (ML^{-3})
SIN -- concentration within biomass (ML^{-3})
slope -- slope of curve in K vs. pH at 20°C
T -- time (hr^{-1})
t -- number of trays
TDS -- total dissolved solids (parts per thousand)
TP -- temperature (°C)
V -- upflow velocity (ft/hr)
VOLCAR -- volume of one carbon particle (m^3)
VR -- contactor volume = total volume of carbon times expansion factor
VS -- superficial velocity (m hr^{-1})
W -- density of water (ML^{-3})
WP -- partial pressure of water vapor (torr)
WTP -- water treatment processes
XK -- constants

SYMBOLS

δB -- thickness of biofilm (m)
δL -- thickness of hydrodynamic film (m)
ϕ -- angle of initial jet to horizontal (°)
θ -- temperature coefficient

SECTION 1

INTRODUCTION

The Toxic Substance Control Act requires that the potential hazard to human health or to the environment must be evaluated before new chemicals are marketed. An effective technique in the process of assessing hazard is the use of mathematical models that predict the transport and transformation of toxic substances in the environment. These models can predict concentrations in air, water, and food on the basis of the characteristics of the toxic substance and of the environment through which it passes. Figure 1 illustrates the exposure routes to man.

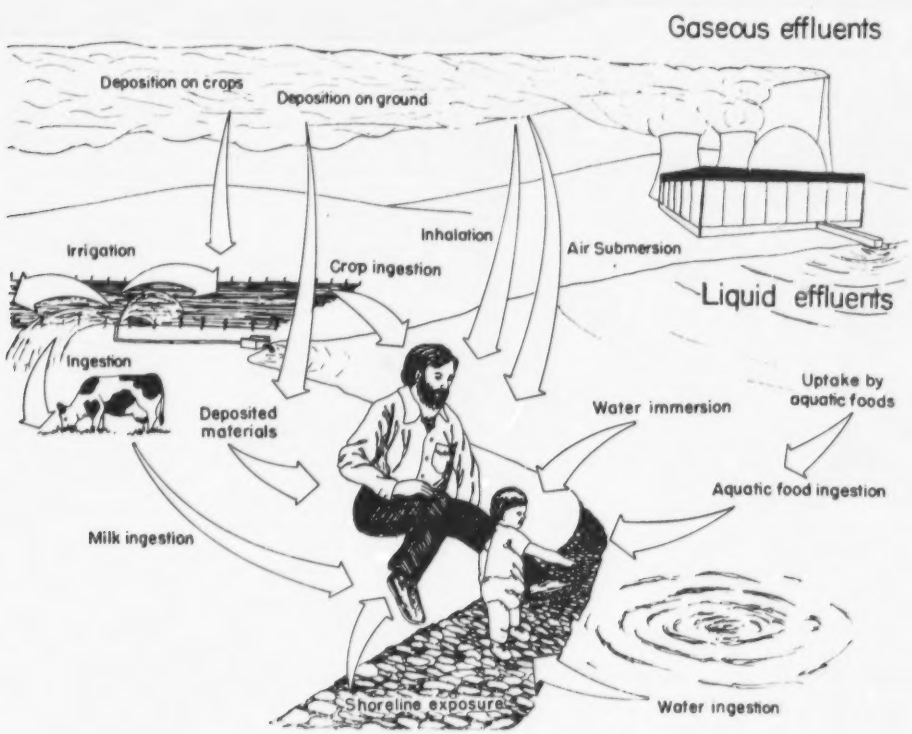

Figure 1. EXPOSURE PATHWAYS TO MAN (After Hoffman et al.)

One important exposure route for humans is the ingestion of chemicals in drinking water. Before reaching humans, these chemicals must pass through municipal water plants where various treatment processes can change the pollutant concentration. An understanding of the transformations and removal processes in the treatment plant linked to information on the transport and transformation of toxic substances in its source waters allow the development of mathematical models that can predict the concentration of a given chemical in drinking water actually at the tap. If the number and distribution of the population at risk is known and human health and toxicological data are available, then the potential hazard of exposure to the chemical can be estimated.

This paper describes a model of municipal water treatment processes for use in predicting the degree of removal of a toxic substance. Removal processes and transformation algorithms for this Water Treatment Processes (WTP) Model are, wherever possible, the same as those used in the model developed by Smith and coworkers at SRI International[1]. Predictions of ambient chemical concentrations using the SRI model may be used as input to the WTP Model.

SECTION 2

CONCLUSIONS

1. A simple mathematical model has been developed that can determine the amount of toxicant removed by various water treatment processes. This model can provide useful predictions of concentration of toxic organic chemicals in finished water.

2. Toxic chemicals that have a high partition coefficient, and hence a high affinity for particulate matter, will be removed by those processes that tend to remove particulate matter.

3. Chemicals that do not readily sorb to particulates are not removed to any appreciable extent unless they volatilize or are reactive. In this case, aeration, chemical oxidation, or carbon adsorption may be effective in reducing a toxicant's concentration in the finished water.

4. In general, for meaningful removal to occur, a compound's halflife must be on the order of one third of the system detention time of the process or system under consideration.

SECTION 3

RECOMMENDATIONS

This work has identified the need for further work in this area. We have developed the following recommendations as a result of our experiences with this exposure assessment model.

1. Obtain more data relating chlorine dosage to trihalomethane formation and to the presence of various organic chemicals. If enough data for a specific chemical are collected, then it should be relatively simple to develop a general regression model for prediction of formation of chlorinated organics.

2. Continue development of models for the description of the removal processes for other water treatment processes, so that a wider variety of water treatment process configurations may be described.

3. Continue refinement on the carbon adsorption process module in order to simplify the data requirements.

4. Link this model to an aquatic fate and transport model, a source identification and loading model, and a model for estimating populations at risk. The actual amount of toxicant reaching a population for consumption in their drinking water could then be predicted.

SECTION 4

MODEL DEVELOPMENT

The Water Treatment Processes Model accepts input data on influent streams, treatment processes, configurations, and appropriate process rate constants for sedimentation, coagulation-flocculation, filtration, aeration, chemical oxidation, adsorption onto granular activated carbon columns, and chlorination. These treatment processes were selected because they are widely used in municipal plants in the United States. The program calls the appropriate process subroutine, i.e., one for each of the treatment processes listed above, in the sequence specified.

Sedimentation

Sedimentation, the oldest process for improving water quality for domestic use, uses subsidence and deposition to separate coagulated or suspended matter from the water. An effective means of water treatment, sedimentation was used in ancient Egypt, Carthage, and Rome[3].

Hazen[4] was the first to show that the floor area (and by analogy surface area) is the primary factor in determining how much suspended material may be removed by a sedimentation basin. Later investigators, including Camp[5], have stated that "for any given discharge, the removal of particles is a function of the surface area and is independent of the depth of the basin; or, the removal is a function of the overflow rate and for a given discharge is independent of the detention period." For the WTP Model, an empirical relationship was established between overflow rate and the removal efficiency of suspended solids, using the same approach as that of Smith[6]. Although few data are available for correlating overflow rate and suspended solids removal efficiency for water treatment, a fair amount of information has been published for wastewater treatment. Using data on removal efficiency of suspended solids versus overflow rate as tabulated and plotted by the American Society of Civil Engineers[7], the expression

$$Sed_{rem} = 0.76 * Sed_{inf} * e^{\frac{-OF}{3247}} \qquad (1)$$

was derived, where the overflow rate (OF) is in gallons per day per square foot of surface area (gpd/ft^2). If sorption of toxics to the suspended solids is taken into account and a mass balance is performed, the toxic substance concentration in the settling basin effluent can be calculated. Sorption is assumed to be completely reversible.

The fraction of the total amount of toxicant associated with particulate matter, defined as F, is determined by the following expression[8],

$$F = \frac{1}{1 + W/(Sed*CP)} \qquad (2)$$

where W is the density of water. This expression can be solved for a range of sediment concentrations (Sed) and partition coefficients (CP) to illustrate the relative importance of particulate matter as a toxicant transport medium[8]. As will be seen later, removal with particulates will be the major means of removal for chemicals sorbed by particulates.

Coagulation-Flocculation

Coagulation, the usual pretreatment before rapid sand filtration, involves the addition of chemicals to water, their uniform distribution through the water, and the buildup of a readily settleable floc. The process involves an initial high speed mix to ensure adequate, prompt dispersion of chemicals in the water; an intermediate mix at lower speed, allowing flocculation and conditioning; and a period to allow sedimentation of the floc. It has been shown[9] that the detention time is more important than the overflow rate in achieving flocculation. Coagulation-flocculation has been modeled for water treatment systems using either conventional coagulation-sedimentation or suspended solids contact clarification. For both cases, the formulations of Wanielista,[10,11] that were empirically derived from data collected by Wanielista and from Kincaid,[12] were adopted for the WTP Model. Again the basic removal equation is an exponential expression:

$$Sed_{eff} = Sed_{inf} * e^{KT} \qquad (3)$$

The required data for the conventional coagulation-sedimentation process are the detention times for the flocculation basin (DTF) in minutes and the sedimentation basin (DTS)in hours. These detention times are used to determine KT (dimensionless) in the removal equation, where

$$K = (-0.062 - (0.07774 * DTF) ** 0.305 * DTS * 2.3).$$

Filtration

In recent years, water has been prepared for filtration in basins that combine mixing, flocculation, conditioning, sedimentation, and sludge removal in a single unit. Coagulation and flocculation take place in the presence of previously formed floc and excess solids are continually removed from the bottom. To model this suspended solids contact clarifier, the only additional parameter needed is the upflow velocity in the clarifier. The upflow velocity determines the efficiency of the clarifier and the surface area determines the upflow velocity. KT is then determined by the expression,

$$KT = -0.891 * Q/V$$

where Q is the influent flow rate in MGD and V is the upflow velocity in ft/hr.

The most common device for treating municipal water supplies is the rapid sand filter, which removes nonsettleable floc and impurities remaining after chemical coagulation and sedimentation of the raw water. Water passes downward through the filter by a combination of positive head and suction from the bottom. The action of the filter is extremely complex, consisting of straining, flocculation, and sedimentation. An exponential formulation adapted from Wanielista[10,11] is used in the WTP Model:

$$Sed_{eff} = XK1 * Sed_{inf}^{XK3} e^{K}, \qquad (4)$$

where: $K = -\frac{(SA * XK2)}{Q}$

More exacting formulations can be developed but they require data that are not readily available.

These processes remove particulate matter. Therefore, those toxic compounds that have a high partition coefficient will be preferentially removed with the particulate matter per equation 2. The following processes will remove the chemicals remaining in solution.

Aeration

Aeration is normally used either to add oxygen to water or remove volatile substances from water. The WTP Model includes spray aeration and multiple tray aeration.

Spray aeration will increase volatilization of a compound, expose it to photodegradation during daylight hours and increase its potential for oxidation[13].

The following expression is used[1, 13, 14].

$$C_{eff} = C_{inf} e^{-KT} \qquad (5)$$

where: $K = \frac{KV + KPD + (K2 * O_2 * 18000^{-1})}{1 + CP * Sed_{inf} * 10^{-7}}$

$$O_2 = \left(\frac{475 - 2.65 * TDS}{33.5 + TP}\right) * \left(\frac{AP - WP}{760 - WP}\right)$$

$$T = 1800^{-1} * CD * \sin\left\{\phi * \sqrt{2h/G}\right\}$$

Scott[15] developed a similar formulation for multiple tray aeration:

$$C_{eff} = C_{inf} * e^{-Kt} \quad (6)$$

where: $K = 0.0608 * \left(\frac{44}{MW}\right)^{1/2}$

t = number of trays

Equation 6 only takes into account volatilization; 44 is the molecular weight of carbon dioxide, which was used as the reference compound because extensive data exist for it. Photodecomposition would not be important here because, unlike spray aeration, multiple tray aerators are almost always enclosed. Oxidation is not included.

Chemical Oxidation

The purpose of oxidation in water treatment is to convert undesirable chemical species to species that are neither harmful or otherwise objectionable. Chemical oxidation processes were used as early as the eighteenth century to control taste and odor problems in drinking water. In those few early instances, simple oxygenation of public water supplies was employed to enhance oxidation of decomposed vegetation and animal matter. This practice did not gain widespread use until the latter half of the nineteenth century, at which time oxygenation of public water supplies had become general practice[15]. As the overall benefits of oxidation and the shortcomings of using atmospheric oxygen became more clearly recognized, attempts were made to use stronger and more effective oxidants such as ozone, permanganate, chlorine dioxide, and chlorine[16]. In the WTP Model, an exponential decay function is again used. Values for the rate constants as a function of hydrogen ion activity (pH) must be determined. A generalized temperature coefficient is used to account for increases in oxidation rate as temperature increases[13].

$$C_{eff} = C_{inf}\, e^{-Kt} \quad (7)$$

where:

$$K = (K2)\, e^{(\text{slope}\ [pH-7])}\, \theta^{(T-20)}\, Conc_{ox}$$

For this equation, data on the 2nd order oxidation rate constant (K2) at different pH values is needed so that both a range and a slope can be developed. Otherwise, measured values for the operating range are required.

Adsorption onto Activated Carbon

Adsorption with activated carbon has traditionally been used to control taste and odor, but, with the advent of regulations for the control of trihalomethanes and other toxic organics, carbon adsorption by granular activated carbon columns will be more widely used. The granular carbon adsorption formulation in the WTP Model is based on the work of Kashel[17] involving wastewater treatment systems. The carbon adsorption model is

based on the premise that an effective lumped parameter model can be formulated. This formulation is possible if the competitive removal mechanisms of adsorption and bio-oxidation are considered to be parallel rather than sequential mechanisms. On this basis, the following mass balance can be made.

$$E * VR * \frac{dC}{dt} = (C_{inf} * Q)-(C_{eff} * Q)-(E * VR * RXC)-(E * VR * RXS) \quad (8)$$

This formulation is restrictive in that it does not allow for competitive adsorption between organics and does not account for byproducts resulting from tranformations. The formulation, however, does allow for biomass sloughing that results in a net increase in suspended solids and particulate organics concentrations across the contactor.

Kinetic formulations developed for RXC and RXS[17] are:

$$RXS = KFB\ (S-SIN) \quad (9)$$

where: $KFB = \frac{KF*NCPC*AB}{VR}$

$$KF = \frac{JD*VS}{NSC^{2/3}}$$

$$JD = 1.34 * \left(\frac{NRE}{1-EPEX}\right)^{-0.468}$$

$$NCPC = \frac{RHOPAC * VR}{RHOCP * VOLCAR * (1-E)}$$

All these parameters are either system-specific or easily calculated.

Film diffusion has been found to be rate-limiting in most applications.

$$RXC = KFA * A\ (S-S^*) \quad (10)$$

where: $$KFA = \frac{1}{\frac{\delta L}{DL} + \frac{\delta B}{DB}}$$

Wen and Yu[18] have established the following equation for activated carbon.

$$EPEX = \left(\frac{13.86\ RHOL^{.4}\ MU^{.6}\ VS^{1.4}}{DCP^{1.6}\ (RHOBC - RHOL)G}\right)^{.18} \quad (11)$$

Having calculated the expanded bed porosity (EPEX), equations 9 and 8 can now be exercised and solved for the steady state effluent concentration.

To accurately simulate the process, S must be estimated as a function of the fixed phase concentration, QE. The relationship between S and QE can be expressed as an isotherm such that S will be zero when QE is zero. An expression of the form

$$QE = b + m^* \log S$$

should give an acceptable prediction equation for S[17], where b is the y intercept and m the slope.

Chlorination

Chlorination is the single most widely used water treatment process in the United States[19]. Disinfection is its most common objective, undoubtedly saving numerous lives by preventing epidemics of water borne disease. Chlorination, however, may also cause formation of toxic cholorinated compounds or may oxidize chemicals in the raw water to more toxic forms. Whether a given compound is changed depends primarily on its oxidation state, with the higher states less likely to change. Insufficient data are available to permit the development of a generalized chlorination model at this time. Rather, each new compound will need to be considered individually for predictive purposes. The extent of any change due to chlorination will depend upon the chlorine dosage, toxicant concentration, and time of contact. Moore et al.[20] developed a regression model relating chlorine dosage to the chloroform concentration in the distribution system. If enough data of this type for a specific chemical are collected, it would be relatively simple to develop a general regression model for that chemical.

SECTION 5

RESULTS AND DISCUSSION

The objective of this effort was to develop a model of water treatment processes that predicts the quantity of a toxicant in the finished water. When such a model is linked to an aquatic fate and transport model, a source identification and loading model, and a model for estimating the population at risk, the amount of toxicant reaching a population for consumption in their drinking water can be predicted. Smith and coworkers[21] developed an aquatic fate and transport computer model and supporting laboratory procedures to measure the sorption partition coefficient and the rate constants for volatilization, oxidation, hydrolysis, photolysis, and microbial transformations, under conditions that are extrapolatable to environmental conditions[1]. Smith and coworkers[21] applied these procedures to 11 toxic chemicals of environmental concern, and used the results with their aquatic fate and transport model to predict the pathways for these chemicals in ponds, lakes and rivers. Their descriptions, coefficients and constants are also used whenever possible as input to the WTP Model.

Table 1 shows the partition coefficients and rate constants for volatilization (KV), photodegradation (KPD), and oxidation (KOX) used for the 11 toxic chemicals modeled by Smith and coworkers[21]. As an example, if the WTP Model is run using the water treatment process train shown in Figure 2

TABLE 1
Rate Constants of 11 Selected Chemicals

Chemical	CP ($X10^{-3}$)	KV ($X10^{4}$ hr^{-1})	KPD ($X10^{2}$ hr^{-1})	KOX ($X10^{5}$ hr^{-1})
p-Cresol	0.01	40	0.05	7
Quinoline	0.01	1	0.06	7
Methyl Parathion	0.05	0.02	0.2	0.35
Benzothiophene	0.05	150	0.06	0.70
9H-Carbazole	0.2	0.07	11	290
Benzoquinoline	1.4	0.08	25	0.01
Dibenzothiophene	1.4	50	0.18	0.70
7H-Dibenzocarbazole	20	0.47	69	100
Benzoanthracene	25	0.07	3.4	1800
Benzopyrene	50	50	23	200
Mirex	300	14	0.009	7

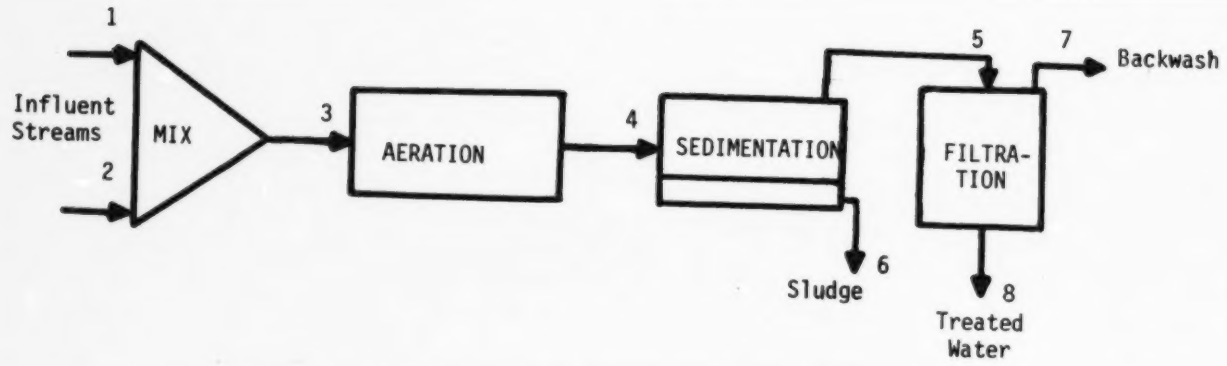

Figure 2. EXAMPLE WATER TREATMENT PROCESS TRAIN

and the partition coefficients and rate constants of Smith et al., the removals shown in Table 2 are obtained for these 11 compounds.

These results illustrate the effect that the partition coefficient (CP) of a toxicant has upon its mechanism of removal in water treatment. Toxic chemicals that have a high partition coefficient, will be removed by those processes that tend to remove particulate matter. Hence, a chemical such as mirex, which is almost completely sorbed to particulates, will be removed at or near the same rate as the particulates. Processes such as sedimentation, coagulation-flocculation, and filtration will be effective in its removal from the product water. A chemical that has a low partition coefficient such as quinoline, however, will be essentially unaffected by those processes that remove particulate material. Consequently, chemicals that do not readily sorb to particulates are not removed unless they undergo some other transformation; in which case, aeration, chemical oxidation, or carbon adsorption may be effective in reducing the toxicant's concentration in the finished water. The detention time of water in a water treatment system is on the order of one day. Therefore, it should be noted that compounds that have halflives significantly greater than the detention time of the system will not be degraded or volatilized. In general for significant degradation to occur, the halflife must be on the order of one third of the system detention time.

Thus, if the influent to the water treatment plant diagrammed in Figure 2 contained 60 ug/l of mirex and 6 g/l of quinoline (the approximate solubility limits), then it would be predicted by the WTP Model that the effluent concentrations would be 3.5 ug/l and 5.4 g/l, respectively. Most of this work has been previously published[22].

Summary

The WTP Model calls subroutines for each of the treatment processes being modeled, an output subroutine and several other supporting subroutines. The process subroutines presently include sedimentation, coagulation-flocculation (two versions), filtration, aeration (two versions), chemical oxidation and granular activated carbon adsorption.

The chlorination subroutine needs more experimental data upon which to base the modeling effort, and in all probability chemicals will need to be modeled on an individual basis. Any specific process can be similarly added for which enough experimental information is available upon which to construct a model algorithm. The WTP Model provides a means of predicting the quantity of a toxic in tap water following treatment. When linked with an aquatic fate and transport model, a source identification and loading model, and a model for estimating the population at risk, the WTP Model can be used to predict the amount of a toxicant actually reaching a population for consumption by the drinking water route.

TABLE 2
Predicted Removals Using WTP Model for
11 Selected Chemicals

CP ($X10^{-3}$)	% Removal With Sediment	K's ($X10^{2}$ hr^{-1})	% Removal in Water Phase	% Removal (Total)
0.01	0.1	0.05	9.1	9.2
0.01	0.1	0.077	9.2	9.3
0.05	0.7	0.2	10.1	10.8
0.05	0.7	1.5	11.8	12.5
0.2	2.9	11	58.4	61.3
1.4	16.7	25	31.8	48.5
1.4	49.6	0.68	3.9	53.5
20	63.0	70	17.0	80.0
25	67.2	5.2	2.6	69.8
50	76.4	24	2.7	79.1
300	80.9	0.14	0.2	81.1

SECTION 6

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APPENDIX A. USERS MANUAL

A digital computer program that can be used to compute the quasi-steady-state concentration of a toxic substance in a typical water treatment process train has been developed. This program is written in FORTRAN and is designed to be run interactively on a DEC PDP 11/70 computer. The program presently consists of a main executive program and nine process subroutines; each subroutine computes the transformation of a toxic substance undergoing a single water treatment process. Three other subroutines are also provided. The first, entitled PER, simply calculates the amount of removal of the toxic substance in each process as percent removed from the water, with the sediment, and total for that process. The second subroutine, entitled PN1, calculates the equilibrium concentration of the toxic substance on the sediment in milligrams of toxic substance per gram of sediment. The third subroutine, entitled PRINT, simply prints all pertinent data. The nine processes presently included in the program together with the subroutine names are listed below:

Process Name	Subroutine Name
Primary sedimentation	SED1
Aeration	AER2
Chemical oxidation	COX3
Coagulation	COAG4
Filtration	FIL5
Granular activated carbon column adsorption	GAC6
Chlorination	THM7
Mixing	MIX
Steam splitting	SPLIT

Program Description

The first step in using the program is to draw the process diagram showing the processes to be used and the connecting and recycle streams. For this purpose the process symbols shown in Figure A-1 are suggested. Example process diagrams are shown in Figure A-2. Each process and each stream is assigned a number by the program user. The processes may be numbered up to 20 and the streams may be numbered up to 30. The principal influent stream to the system is assigned the number one and the principal effluent stream from the system is assigned the highest stream number used. The number zero is given to processes involving no decision variables, such as in mixing or stream splitting.

The program provides for initially reading in up to ten influent and recycle streams as input. All stream vectors are stored in the stream matrix (XM), which has 8 rows and 30 columns. One stream vector is stored

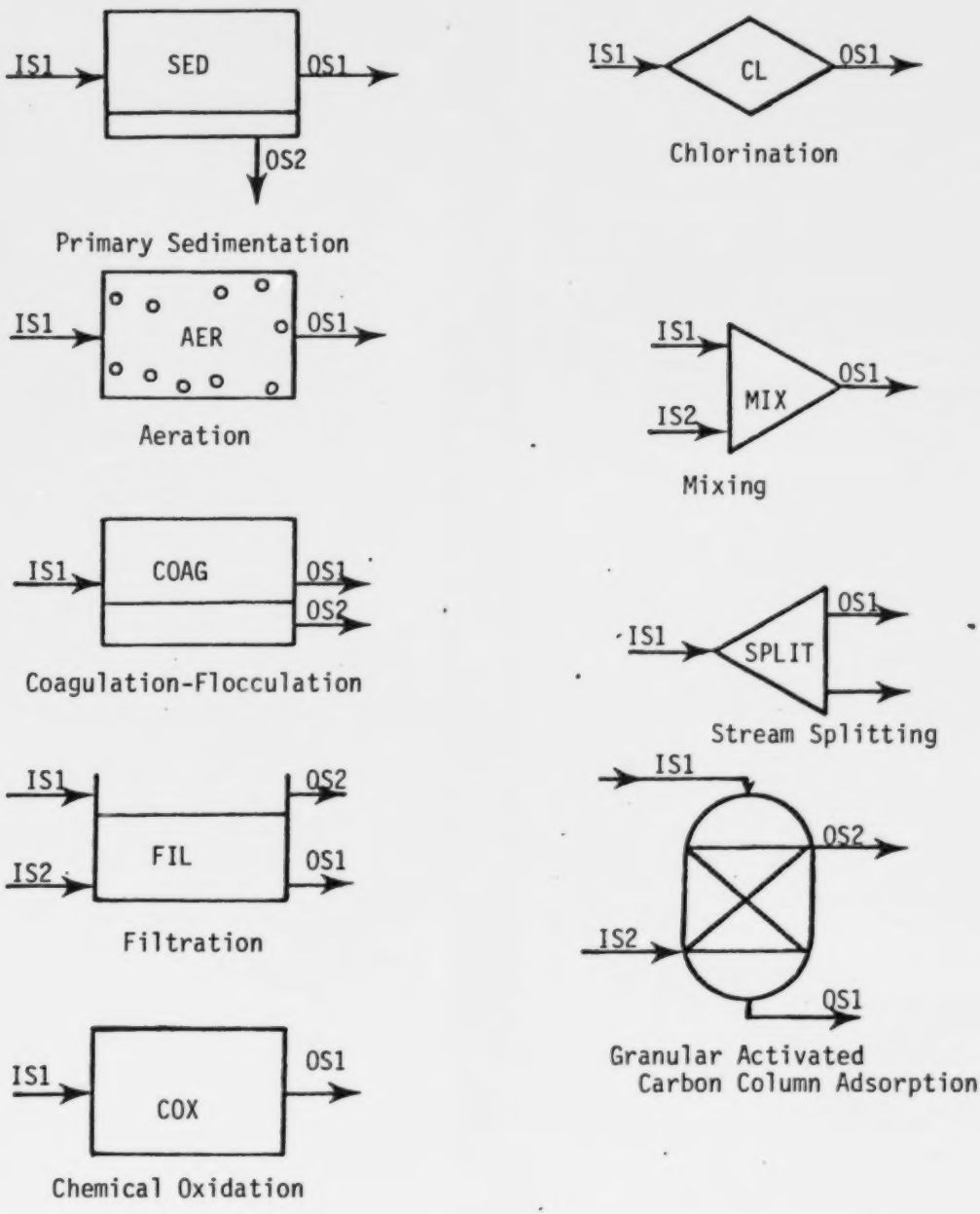
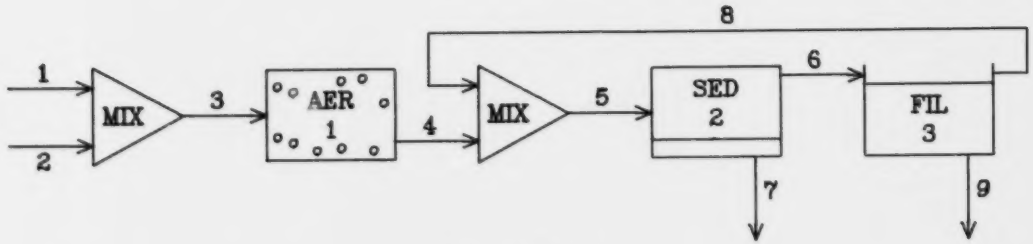
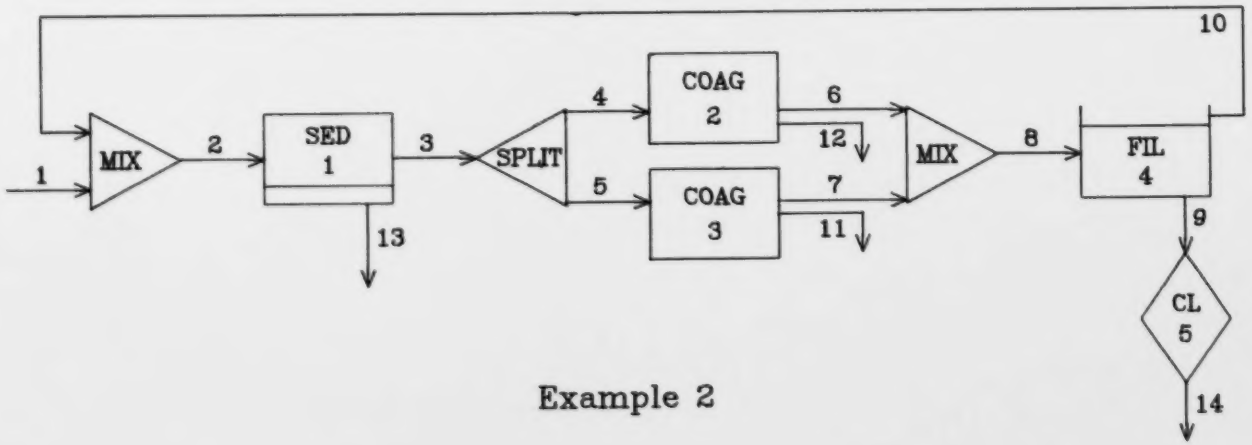


Figure A-1. PROCESS SYMBOLS



Example 1



Example 2

Figure A-2. EXAMPLE PROCESS FLOW DIAGRAM

in each column of XM. A temporary stream matrix (TXM) with 8 rows and 30 columns is used internally by the program to store newly computed stream vectors until they can be compared with the previously computed values during the program recycle iterations. The acceptable error (TIT), which will be tolerated when recycle streams are involved, is also supplied as input to the program. Each stream is described by the stream number in the first row of XM, the volume flow in million of gallons per day (MGD) in the second row, the suspended sediment load in milligrams per liter in the third row, the amount of toxic substance per unit weight of sediment in milligrams per gram in the fourth row, and the concentration of the given toxic substance in micrograms per liter in the fifth row. Subsequent rows may be used for other contaminants as new process subroutines are added to the program or modifications are made in the existing ones. A list of the information contained in the present stream vectors are shown in Table A-1 with the FORTRAN variable names used.

Two decision matrices (XK, 20 rows and 12 columns; XS, 20 rows and 3 columns) are provided for storing design parameters such as surface area or detention times. The XK matrix is process specific. The XS matrix contains parameters common to two or more processes, such as the density of water, or of a sediment, or a partition coefficient. Decision parameters for the Nth process are stored in the Nth row of XK. A list of the contents of XK and XS are shown in Table A-2.

The main program is entitled MAINE and calls the process subroutines for computing the performance of the individual processes.

Table A-1
Contents of Stream Matrix (XM)
(I designates the stream number)

Row No.	Descriptive Parameter	FORTRAN Variable Name
1	Stream Number	XM (1, I), I
2	Volume Flow, MGD	XM (2, I), Q
3	Suspended Sediment, mg/l	XM (3, I), SED
4	Toxic Substance Sorbed to Sediment, mg/g	XM (4, I), XM
5	Dissolved Toxic Substance, ug/l	XM (5, I), CON
6	Unassigned	
7	Unassigned	
8	Unassigned	

Table A-2
Contents of Decision Matrix
(PN designates the process number)

Primary sedimentation

XK (PN, 1) = DEP = depth (ft)
XK (PN, 2) = SA = surface area (1000 ft^2)
XK (PN, 3) = F = fraction of influent to underflow
XK (PN, 4) = OF = overflow rate of sedimentation basin (gal ft^{-2} day^{-1})
XK (PN, 5) = DT = detention time of sedimentation basin (hr)

Aeration

XK (PN, 1) = AP = atmospheric pressure (torr)
XK (PN, 2) = OP = oxygen vapor pressure (torr)
XK (PN, 3) = TEMP = temperature (°C)
XK (PN, 4) = TDS = total dissolved solids (mg/l)
XK (PN, 5) = CPD = photolysis rate constant (hr^{-1})
XK (PN, 6) = COX = pseudo first order rate constant for oxidation (hr^{-1})
XK (PN, 7) = CV = mass transfer rate constant for volatilization (hr^{-1})
XK (PN, 8) = DT2 = detention time (hr)
XK (PN, 9) = SMT = selector-spray = 0, multiple tray = 1
XK (PN, 10) = XMW = molecular weight of chemical
XK (PN, 11) = XNT = number of trays

Chemical oxidation

XK (PN, 1) = XK2 = second order rate constant ($1M^{-1}Min^{-1}$) at 20°C and pH 7
XK (PN, 2) = SLOPE = slope of K vs pH curve at 20°C
XK (PN, 3) = PH = pH
XK (PN, 4) = THETA = constant for temperature correction of rate constant
- here 1.047
XK (PN, 5) = CONX = concentration of oxidant (M/l)
XK (PN, 6) = TEMP = temperature (°C)
XK (PN, 7) = DT3 = detention time (min)

Coagulation-flocculation

XK (PN, 1) = DTF = flocculation basin detention time (min)
XK (PN, 2) = DTS = sedimentation basin detention time (hrs)
XK (PN, 3) = FUF = fraction underflow
XK (PN, 4) = SSCC = selector-conventional = 0, SSCC = 1
XK (PN, 5) = UV = upflow velocity (ft/hr)

Filtration

XK (PN, 1) = SA = surface area (100 ft^2)
XK (PN, 2) = XK1 = constant = 2.303
XK (PN, 3) = XK2 = constant = 1.244
XK (PN, 4) = XK3 = constant = 0.81

Table A-2 (cont'd.). Contents of Decision Matrix

Granular activated carbon

XK (PN, 1) = DBIO = thickness of biomass on a carbon particle (m)
XK (PN, 2) = AREA = cross-sectional area of contactor (cm^2)
XK (PN, 3) = CARBON = volume of carbon per contactor (m^3)
XK (PN, 4) = DL = diffusivity of chemical in water ($m^2\ hr^{-1}$)

Chlorination

XK (PN, 1) = FCL = rate constant (hr^{-1})

Common processes

XS (1,3) = CP = partition coefficient
XS (1,1) = DENW = density of water in g/cc (defalt 1.0)
XS (1,2) = DENS = density of sediment in g/cc (defalt 1.2)
XS (IS1,1) = fraction of stream IS1 split to stream OS2 (defalt .5)

This program is interactive. The initial prompt will be NCASE? (Figure A-3). The number of runs the user wishes to make should be entered. This is followed by CHEMICAL?. The name of the chemical the user wishes to model is entered. The next prompt is TOLERENCE, NO. OF INPUT STREAMS, & STREAM NOS?. Tolerence refers to TIT, the fractional varience allowed between iterative calculations. The number of input streams and stream numbers are self explanatory. This is followed by prompts for entry of stream variables for each influent stream. A description of the system configuration, i.e., the processes to be used and the location of the interconnecting streams, is communicated to the computer for each process at the prompt K, PN, IPROC, IS1, IS2, OS1, OS2, & LK?. The control integer K designates process loops, K = 0 (no branch), K = 1 (branch point) and K = 9 (end of file for input). The integer PN is the process number, which is sequentially assigned to each process. The process identification number IPROC identifies the type of process and the corresponding subroutine. The process subroutine name and its corresponding identification number are:

Subroutine Name	IPROC
SED1	1
AER2	2
COX3	3
COAG4	4
FIL5	5
GAC6	6
THM7	7
MIX	10
SPLIT	11

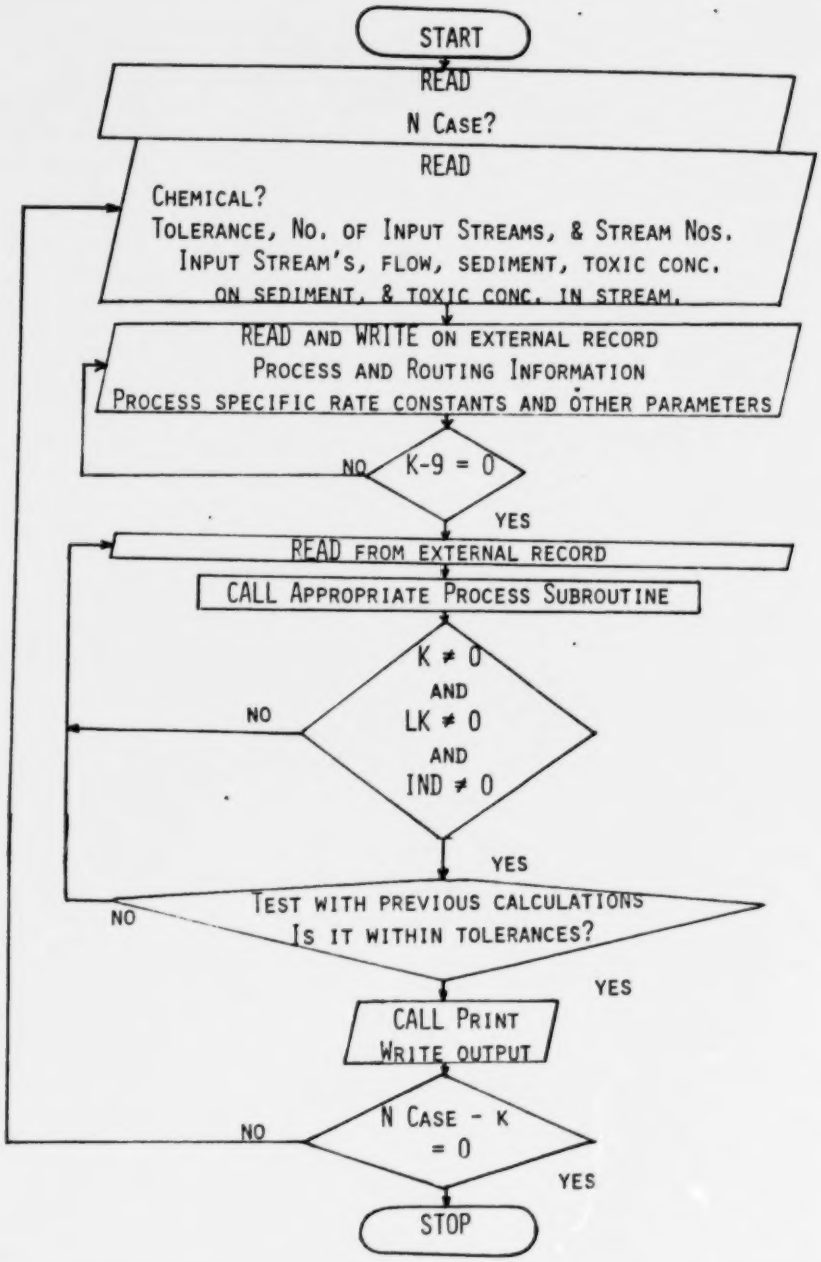


Figure A-3. PROGRAM FLOW CHART

The number of the principal input stream to the process (IS1) is entered. If a second input stream exists, the number of the stream (IS2) is entered, otherwise enter 0. The principal output stream from the process (OS1) is entered. If a second output stream exists, the number of the stream (OS2) is entered, otherwise enter 0. The control integer LK designates processes not in any loop, LK = 0 (not in any loop), LK = 1 (in loop), and LK = 9 (last process). The next prompt is PROCESS (PN), PROCESS RATE CONSTANTS? or RATE CONSTANTS? if mix was specified or SPLIT? if SPLIT was specified. Enter the appropriate decision variables (Table A-2) for the given process and specified chemical, followed by -1. Note that every line of input is terminated by / and a carriage return.

The last two prompts will repeat until all processes have been described, at which point a K = 9 is entered as previously described to indicate input end of file. Sample input is shown in Figure A-4 for the process configuration shown in Figure A-2.

Printed output format

Sample output for the program is shown in Figure A-5. The input is that shown in Figure A-4. The first table shows the input process and routing data that describe the water treatment system that was simulated. The second table shows selected input process rate constants supplied for each process.

The third output table lists the calculated steady state stream characteristics by stream number. The stream characteristics listed are, Q, volume flow in million gallons per day (MGD); SED, suspended sediment concentration in milligrams per liter (mg/l); XM, amount of chemical on the sediment, in milligrams chemical per gram sediment (mg/g); and CON, the concentration of chemical in the water in micrograms per liter (ug/l).

The last output table lists the processes according to the process number and gives the name of the process along with all pertinent parameters relating to the process. The process is identified by the letter P, followed by the process number in the left hand column of the printout, e.g., process number 2 is identified by P2. The percent of the chemical removed with the sediment, the amount disappearing from the aqueous phase and the total amount of chemical removed from the water column is also shown for each process. This is followed by this same removal data for the water treatment process chain as a whole.

Table A-3 defines FORTRAN symbols used in the program.

```
PDS> RUN MAINE
08:39:43
NCASE?2
CHEMICAL?METHYL PARATHION

TOLERENCE,NO.OF INPUT STREAMS,&STREAM NOS?
.01 2 1 2/

INPUT STREAM NO. 1  FLOW,SED,XM,&CON?
1 100 1 300/

INPUT STREAM NO. 2 FLOW,SED,XM,&CON?
.5 300 .5 100/

K,PN,IPROC,IS1,IS2,OS1,OS2,&LK?
0 0 10 1 2 3 0 0/

RATE CONSTANTS?
1 1.2 50 -1/
PROCESS MIX

K,PN,IPROC,IS1,IS2,OS1,OS2,&LK?
0 1 2 3 0 4 0 0/

PROCESS 1 PROCESS RATE CONSTANTS?
760 17.5 20 100 2.E-3 3.5E-6 2.E-6 2 0 -1/

K,PN,IPROC,IS1,OS2,OS1,OS2,&LK?
1 0 10 4 8 5 0 1/
PROCESS MIX

K,PN,IPROC,IS1,IS2,OS1,OS2,&LK?
0 2 1 5 0 6 7 1/

PROCESS 2 PROCESS RATE CONSTANTS?
7 5 .05 0 -1/

K,PN,IPROC,IS1,IS2,OS1,OS2,&LK?
1 3 5 6 0 9 8 9/

PROCESS 3 PROCESS RATE CONSTANTS?
5 2.303 1.244 .81 -1/

K,PN,IPROC,IS1,IS2,OS1,OS2,&LK?
9/

ANY CHANGES IN
CHEMICAL?
 IF NO, TYPE 0, IF YES, TYPE 1  0
```

Figure A-4. EXAMPLE INTERACTIVE RUN

```
ANY CHANGES IN

TOLERENCE,NO.OF INPUT STREAMS,&STREAM NOS?
 IF NO, TYPE 0, IF YES, TYPE 1  1

TOLERENCE,NO.OF INPUT STREAMS,&STREAM NOS?
.01 1 1/

INPUT STREAM NO. 1  FLOW,SED,XM,&CON?
1 100 1 400/

K,PN,IPROC,IS1,IS2,OS1,OS2,&LK?
1 0 10 1 10 2 0 1/

ANY CHANGES IN

RATE CONSTANTS?
 IF NO, TYPE 0, IF YES, TYPE 1  0
PROCESS MIX

K,PN,IPROC,IS1,IS2,OS1,OS2,&LK?
0 1 1 2 0 3 13 1/

ANY CHANGES IN

PROCESS 1  PROCESS RATE CONSTANTS?
 IF NO, TYPE 0, IF YES, TYPE 1  1

PROCESS 1  PROCESS RATE CONSTANTS?
7 5 .05 0 -1/

K,PN,IPROC,IS1,IS2,OS1,OS2,&LK?
0 0 11 3 0 4 5 1/

PROCESS SPLIT
SPLIT?.4

K,PN,IPROC,IS1,IS2,OS1,OS2,&LK?
0 2 4 4 0 6 12 1/

ANY CHANGES IN

PROCESS 2  PROCESS RATE CONSTANTS?
 IF NO, TYPE 0, IF YES, TYPE 1  1

PROCESS 2  PROCESS RATE CONSTANTS?
60 4 .01 0 -1/
```

Figure A-4 (cont'd). EXAMPLE INTERACTIVE RUN

```
K,PN,IPROC,IS1,IS2,OS1,OS2,&LK?
0 3 4 5 0 7 11 1/

ANY CHANGES IN

PROCESS 3  PROCESS RATE CONSTANTS?
 IF NO, TYPE 0, IF YES, TYPE 1  1

PROCESS 3  PROCESS RATE CONSTANTS?
50 4.5 .01 0 -1/

K,PN,IPROC,IS1,IS2,OS1,OS2,&LK?
0 0 10 6 7 8 0 1/
PROCESS MIX

K,PN,IPROC,IS1,IS2,OS1,OS2,&LK?
1 4 5 8 0 9 10 1/

ANY CHANGES IN

PROCESS 4  PROCESS RATE CONSTANTS?
 IF NO, TYPE 0, IF YES, TYPE 1  1

PROCESS 4  PROCESS RATE CONSTANTS?
5 2.303 1.244 .81 -1/

K,PN,IPROC,IS1,IS2,OS1,OS2,&LK?
0 5 7 9 0 14 0 9/

ANY CHANGES IN

PROCESS 5  PROCESS RATE CONSTANTS?
 IF NO, TYPE 0, IF YES, TYPE 1  1

PROCESS 5  PROCESS RATE CONSTANTS?
.05 01/

K,PN,IPROC,IS1,IS2,OS1,OS2,&LK?
9/
JOB533  --  STOP
```

Figure A-4 (cont'd). EXAMPLE INTERACTIVE RUN

INPUT DATA

K	PN	PROCESS	IS1	IS2	OS1	OS2	LK
0	0	10	1	2	3	0	0
0	1	2	3	0	4	0	0
1	0	10	4	0	5	0	1
0	2	1	5	0	6	7	1
1	3	5	6	0	9	8	9

PROCESS RATE CONSTANTS FOR METHYL PARATHION

PN					
1	760.000	17.5000	20.0000	100.000	0.200000E-02
	0.350000E-05	0.200000E-05	2.00000	0.000000	
2	7.00000	5.00000	0.500000E-01	311.833	
3	5.00000	2.30300	1.24400	0.810000	

Figure A-5. EXAMPLE OUTPUT

STREAM CHARACTERISTICS

VOLUME FLOW, MILLIONS OF GALLONS PER DAY
SEDIMENT, MILLIGRAMS PER LITRE
METHYL PARATHION
CONCENTRATION ON SEDIMENT, MILLIGRAMSPER GRAM
CONCENTRATION, MICROGRAMS PER LITRE

STREAM 1.	Q 1.000	SED 100.000	XM 0.1500E-01	CON 300.0000
STREAM 2.	Q 0.500	SED 300.000	XM 0.5001E-02	CON 100.0000
STREAM 3.	Q 1.500	SED 166.667	XM 0.1167E-01	CON 233.3333
STREAM 4.	Q 1.500	SED 166.667	XM 0.1162E-01	CON 232.4024
STREAM 5.	Q 1.559	SED 221.313	XM 0.1162E-01	CON 232.4024
STREAM 6.	Q 1.481	SED 73.181	XM 0.1162E-01	CON 232.4025
STREAM 7.	Q 0.078	SED 3035.818	XM 0.1165E-01	CON 232.3302
STREAM 8.	Q 0.059	SED 1712.897	XM 0.1164E-01	CON 232.4025
STREAM 9.	Q 1.422	SED 4.860	XM 0.1162E-01	CON 232.4025

Figure A-5 (cont'd). EXAMPLE OUTPUT

PROCESS CHARACTERISTICS

	PERCENT REMOVAL						
P 1AERATION	SED	WATER	TOTAL	KPD	KOX	KV	DT
	0.000	0.396	0.396	0.2000E-02	0.3500E-05	0.2000E-05	2.000
P 2PLAIN SEDIMENTATION	SED	WATER	TOTAL	SA	CP	OF	DT
	0.751	4.95	5.70	5.000	50.00	311.8	4.030
P 3FILTRATION	SED	WATER	TOTAL	SA	K1	K2	K3
	0.341	3.99	4.33	5.000	2.303	1.244	0.8100

METHYL PARATHION
PERCENT REMOVAL WITH SEDIMENT= 0.8038
PERCENT REMOVAL IN THE AQUEOUS PHASE= 5.535
TOTAL REMOVAL = 6.339 PERCENT

Figure A-5 (cont'd). EXAMPLE OUTPUT

INPUT DATA

K	PN	PROCESS	IS1	IS2	OS1	OS2	LK
1	0	10	1	10	2	0	1
0	1	1	2	0	3	13	1
0	0	11	3	0	4	5	1
0	2	4	4	0	6	12	1
0	3	4	5	0	7	11	1
0	0	10	6	7	8	10	1
1	4	5	8	0	9	10	1
0	5	7	9	0	14	0	0

PROCESS RATE CONSTANTS FOR METHYL PARATHION

PN					
1	7.00000	5.00000	0.500000E-01	207.807	
2	60.0000	4.00000	0.100000E-01	0.000000	
3	50.0000	4.50000	0.100000E-01	0.000000	
4	5.00000	2.30300	1.24400	0.810000	
5	0.500000E-01	1.00000	0.000000	0.000000	0.000000
	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	0.000000			

Figure A-5 (cont'd). EXAMPLE OUTPUT

STREAM CHARACTERISTICS

VOLUME FLOW, MILLIONS OF GALLONS PER DAY
SEDIMENT, MILLIGRAMS PER LITRE
METHYL PARATHION
CONCENTRATION ON SEDIMENT, MILLIGRAMSPER GRAM
CONCENTRATION, MICROGRAMS PER LITRE

STREAM 1.	Q 1.000	SED 100.000	XM 0.2000E-01	CON 400.0000
STREAM 2.	Q 1.039	SED 97.425	XM 0.2000E-01	CON 400.0000
STREAM 3.	Q 0.987	SED 29.926	XM 0.2000E-01	CON 400.0000
STREAM 4.	Q 0.592	SED 29.926	XM 0.2000E-01	CON 400.0000
STREAM 5.	Q 0.395	SED 29.926	XM 0.2000E-01	CON 400.0000
STREAM 6.	Q 0.586	SED 1.392	XM 0.2000E-01	CON 400.0000
STREAM 7.	Q 0.391	SED 1.105	XM 0.2000E-01	CON 400.0000
STREAM 8.	Q 0.977	SED 1.277	XM 0.2000E-01	CON 400.0000
STREAM 9.	Q 0.938	SED 0.021	XM 0.2000E-01	CON 400.0000
STREAM 10.	Q 0.039	SED 31.429	XM 0.2000E-01	CON 400.0000
STREAM 11.	Q 0.004	SED 2883.196	XM 0.2004E-01	CON 399.8779
STREAM 12.	Q 0.006	SED 2854.703	XM 0.2004E-01	CON 399.8806
STREAM 13.	Q 0.052	SED 1379.919	XM 0.2002E-01	CON 399.9722
STREAM 14.	Q 0.938	SED 0.021	XM 0.2103E-01	CON 420.5085

Figure A-5 (cont'd). EXAMPLE OUTPUT

PROCESS CHARACTERISTICS

P 1PLAIN SEDIMENTATION	PERCENT REMOVAL SED	WATER	TOTAL	SA	CP	OF	DT
	0.343	4.98	5.32	5.000	50.00	207.8	6.048
P 2COAGULATION-FLOCCULATION	PERCENT REMOVAL SED	WATER	TOTAL	TF	TS	FUF	
	0.143	0.999	1.14	60.00	4.000	0.1000E-01	
P 3COAGULATION-FLOCCULATION	PERCENT REMOVAL SED	WATER	TOTAL	TF	TS	FUF	
	0.144	0.998	1.14	50.00	4.500	0.1000E-01	
P 4FILTRATION	PERCENT REMOVAL SED	WATER	TOTAL	SA	K1	K2	K3
	0.629E-02	4.00	4.01	5.000	2.303	1.244	0.8100
P 5CHLORINATION	PERCENT REMOVAL SED	WATER	TOTAL	K1	K2	K3	DT
	-0.538E-05	-5.13	-5.13	0.5000E-01	1.000	0.0000	0.0000

METHYL PARATHION
PERCENT REMOVAL WITH SEDIMENT= 0.4847
PERCENT REMOVAL IN THE AQUEOUS PHASE= 5.058
TOTAL REMOVAL = 5.543 PERCENT

Figure A-5 (cont'd). EXAMPLE OUTPUT

TABLE A-3

Definition of FORTRAN Symbols

Computer Symbol	Definitions and Comments
ACTD	Maximum active thickness of biofilm on carbon particles (m)
AP = XK (PN, 1)	Atmospheric pressure (torr)
AREA = XK (PN, 2)	Cross-sectional area of carbon adsorption contactor (m^2)
BSTAR	Adsorbed phase concentration of chemical (mg l^{-1})
CARBON = XK (PN, 3)	Volume of carbon per contactor (m^3)
CHEM (I)	Name of toxic chemical being modeled
CON = XM (5, IS)	Toxic chemical concentration in aqueous phase of stream number IS (ug l^{-1})
CONX = XK (PN, 5)	Concentration of oxidant in chemical oxidation (M l^{-1})
COX = XK (PN, 6)	Pseudo first order rate constant for oxidation for aeration (hr^{-1})
CP = XS (1,3)	Partition coefficient
CPD = XK (PN, 5)	Photolysis rate constant fo: aeration (hr^{-1})
CV = XK (PN, 7)	Mass transfer rate constant for volatilization in aeration (hr^{-1})
DCP	Diameter of carbon particle (m)
DENBC	Combined density of carbon and biomass (mg l^{-1})
DENBIO	Density of biomass (mg l^{-1})
DENCP	Density of carbon per unit carbon volume (mg l^{-1})
DENPAC	Mass of carbon per unit contactor volume (mg l^{-1})
DENS	Density of suspended sediment particles (g cm^{-3})
DENW	Density of water (g cm^{-3})
DEP = XK (PN,1)	Depth of sedimentation basin (ft)
DL	Diffusivity of chemical in water (m^2 hr^{-1})
DT = XK (PN, 5)	Detention time of sedimentation basin (hrs)
DT2 = XK (PN, 8)	Detention time of aeration basin (hrs)
DT3 = XK (PN, 7)	Detention time for oxidation (min)
DTF = XK (PN, 1)	Detention time for mixing chamber (min)
DTS = XK (PN,2)	Detention time for flucculation basin (hrs)
EPS	Packed carbon bed porosity
EPSI	Expanded carbon bed porosity
F = XK (PN, 3)	Fraction of influent to underflow of sedimentation basin
FPRC	Percent removal of chemical in aqueous phase by treatment system
FPRS	Percent removal of sediment by treatment system

TABLE A-3 (cont'd). Definition of FORTRAN Symbols

FPT	Total percent removal of chemical by treatment system
FR	Fraction of sediment removed in sedimentation basin
FUF = XK (PN, 3)	Fraction underflow from flocculation basin
G	Acceleration due to gravity (m hr^{-2})
GAMMA	Kinematic viscosity of water (m^2 hr^{-1})
INP	Number of input device
IOP	Number of output device
IOSF	Output stream number (OS1) from last process
IP (PN)	Integer matrix that associates the appropriate type process with each process number PN
IPN	Process number of last process
IPROC	Integer input to the program that is used to identify the type of process
IS	Integer input to the program that specifies the number of influent and guess streams to be read by the program
ISF	Input stream number (IS1) from last process
IS1	Input stream number 1 to a process
IS2	Input stream number 2 to a process
K	Integer input to the program that controls recycling in the system. Branch points are designated by K = 1, and end of data by K = 9
K1, K2, K3 = XK (PN, 2, 3, 4)	Constants for filtration, which are equal to 2.303, 1.244, 0.81, respectively
KB	Film rate constant (m^3 mg^{-1} hr^{-1})
KF	Overall bio-oxidation rate constant (m hr^{-1})
KFA	Adsorption mass transfer coefficient (m hr^{-1})
KFB	Biofilm mass transfer coefficient (m hr^{-1})
KFC	Hydrodynamic film mass transfer coefficient (m hr^{-1})
LK	Integer input to the program that controls recycling in the system. LK = 1 designates process is in a loop, LK = 9 designates last process
MAXD	Maximum film thickness
NAS	Integer input to the program that controls acceptance of new input values for NCASE
NCASE	Integer input to the program designating the number of different cases to be executed at a single sitting
NCPC	Number of carbon particles per contactor
NRE	Modified Reynold's number
NSC	Schmidt number
NN (I)	Integer input to the program that specifies the stream numbers of the influent and guess streams to be read by the program

TABLE A-3 (cont'd). Definition of FORTRAN Symbols

NP (PN)	Identifies number of decision variables for process PN
OF = XK (PN, 4)	Overflow rate of sedimentation basin (gal ft^{-1} day^{-1})
OP = XK (PN, 2)	Oxygen vapor pressure for aeration (torr)
OS1	Output stream number 1 from a process
OS2	Output stream number 2 from a process
PE	Fractional expansion of carbon contactor
PH	pH, standard units
PN	Process number assigned to a particular process in the system by the program user
PRC (PN)	Percent removal of chemical with aqueous phase in process number PN
PRS (PN)	Percent removal of chemical with sediment in process number PN
PT (PN)	Percent removal of chemical in process number PN
RXC	Rate of chemical removal by adsorption (g m^{-3} hr^{-1})
RXS	Rate of chemical removal by bio-oxidation (g m^{-3} hr^{-1})
Q = XM (2, IS)	Volume flow of stream number IS, (MGD)
SA = XK (PN, 2)	Surface area of sedimentation basin (1000 ft^2)
SAF = XK (PN, 1)	Surface area of filter (100 ft^2)
SED = XM (3, IS)	Suspended sediment concentration in stream number IS (mg l^{-1})
SMAX	Chemical concentration at which mass transfer no longer limits (mg l^{-1})
SINT	Internal biomass chemical concentration (mg l^{-1})
SLOPE = XK (PN, 2)	Slope of K vs pH curve at 20°C for chemical oxidation
SLUF	Integer variable controlling sluffing of biomass from carbon contactor
SMT = XK (PN, 9)	Integer selector for type of aeration - spray = 0, multiple tray = 1
SSCC = XK (PN, 4)	Suspended solids contact clarifier integer selector - conventional = 0, SSCC = 1
TDS	Total dissolved solids (mg l^{-1})
TEMP	Temperature (°C)
THETA	Constant for temperature correction of rate constant
THETX	Dummy variable
TIT	Iteration tolerance for recycling systems
TXM (I, J)	Temporary stream matrix vector for the Jth stream that is used internally by the program for the recycling iteration
UV = XK (PN, 5)	Upflow velocity in solids contact clarifier (ft hr^{-1})
VOLACT	Maximum volume of biomass (m^3)

TABLE A-3 (cont'd). Definition of FORTRAN Symbols

VOLBIO	Volume of biomass (m^3)
VOLCAR	Volume of one carbon particle (m^3)
VSA	Superficial velocity (m hr^{-1})
XAV	Biomass concentration (g m^{-3})
XK (PN, J)	Decision matrix vector for the Jth variable of process PN
XK2 = XK (PN, 1)	Second order rate constant at 20°C and pH) for chemical oxidation ($1M^{-1}$ min^{-1})
XM = XM (4, I)	Chemical sorbed to sediment in stream number I (mg /g)
XM (I, J)	Stream matrix vector for the Ith variable of stream number J
XMW	Molecular weight of chemical
XNT	Number of trays in aerator
XS (I, J)	Decision matrix vector common to more than one process
Y	Yield coefficient

APPENDIX B: PROGRAM LISTING

```
FORTRAN IV-PLUS V3.0              08:50:18    12-JUN-81          PAGE 1
MAINE,FTN;326          /CK/TR:ALL/WR

      C         MAINE PROGRAM
0001            DIMENSION NN(10),NP(20)
0002            INTEGER IS1,IS2,OS1,OS2,PN
0003            COMMON /C/CHEM(20)
0004            COMMON /XSH/XS(20,3)
0005            COMMON /IO/IOP,INP
0006            COMMON /IFP/ISF,IOSF
0007            COMMON XM(8,30),TXM(8,30),IP(20),
     1          IS1,IS2,OS1,OS2,XK(20,12),PRS(20),PRC(20),PT(20),PN
0008            DEFINE FILE 4 (50,15,U,NWNNN)
0009            INP=5
0010            IOP=6
0011            WRITE(INP,5)
0012       5    FORMAT(' NCASE?',8)
0013            READ(INP,*)NCASE
0014            DO 1000 ILL=1,NCASE
0015            DO 10 I=1,20
0016            DO 9 JJ=1,3
0017       9    IF(ILL .EQ. 1)XS(I,JJ)=0.
0018            DO 10 J=1,8
0019            IF(ILL .EQ. 1)XK(I,J)=0.
0020            DO 10 N=1,30
0021            TXM(J,N)=0.
0022      10    IF(ILL .EQ. 1)XM(J,N)=0.
0023            KKK=1
0024            K=0
0025            IND=0
0026            IBAD=0
0027            LK=0
0028            IF(ILL .EQ. 1)GOTO 101
0029      20    FORMAT('0ANY CHANGES IN',8)
0030            WRITE(INP,20)
0031            WRITE(INP,102)
0032            WRITE(INP,30)
0033      30    FORMAT('  IF NO, TYPE 0, IF YES, TYPE 1  ',8)
0034            READ(INP,50)NAS
0035      50    FORMAT(I2)
0036            IF(NAS .EQ. 0)GOTO 104
0037     101    WRITE(IAP,102)
0038     102    FORMAT(' CHEMICAL?',8)
0039            READ(INP,103)CHEM
0040     103    FORMAT(20A2)
0041     104    CONTINUE
0042            IF(ILL .EQ. 1)GOTO 105
0043            WRITE(IAP,20)
0044            WRITE(INP,106)
0045            WRITE(INP,30)
0046            READ(INP,50)NAS
0047            IF(NAS .EQ. 0)GOTO 115
0048     105    WRITE(IAP,106)
0049     106    FORMAT('0TOLERENCE,NO.OF INPUT STREAMS,&STREAM NOS?',8)
0050            READ(INP,*)TIT,IS,(NN(I),I=1,IS)
0051            DO 115 J=1,IS
0052            KK=NN(J)
0053            WRITE(INP,107)KK
0054     107    FORMAT('0INPUT STREAM NO.',I2,2X,'FLOW,BED,XM,&CON?',8)
```

```
0055      108     READ(INP,*)(XM(I,KK),I=2,5)
0056      115     CONTINUE
0057      120     WRITE(INP,125)
0058      125     FORMAT('0K,PN,IPROC,IS1,IS2,OS1,OS2,LK?',8)
0059              READ(INP,*)K,PN,IPROC,IS1,IS2,OS1,OS2,LK
0060      134     CONTINUE
0061              IF((K-9) .EQ. 0)GOTO 200
0062              XM(1,IS1)=IS1
0063              XM(1,OS1)=OS1
0064              IF(IS2 .EQ. 0)GOTO 140
0065              XM(1,IS2)=IS2
0066      140     IF(OS2 .EQ. 0)GOTO 152
0067              XM(1,OS2)=OS2
0068      152     IF(IS1 .NE. 1)GOTO 159
0069      155     IF(ILL .EQ. 1)GOTO 157
0070              WRITE(INP,20)
0071              WRITE(INP,158)
0072              WRITE(INP,30)
0073              READ(INP,50)NAS
0074              IF(NAS .EQ. 0)GOTO 159
0075      157     WRITE(INP,158)
0076      158     FORMAT('0RATE CONSTANTS?',8)
0077              READ(INP,*)XS(1,1),XS(1,2),XS(1,3)
0078      159     IF(PN .EQ. 0)GOTO 190
0079              IP(PN)=IPROC
0080              IF(ILL .EQ. 1)GOTO 160
0081              WRITE(INP,20)
0082              WRITE(INP,167)PN
0083              WRITE(INP,30)
0084              READ(INP,50)NAS
0085              IF(NAS .EQ. 0)GOTO 200
0086      160     WRITE(INP,167)PN
0087      167     FORMAT('0PROCESS',I2,2X,'PROCESS RATE CONSTANTS?',8)
0088              READ(INP,*)(XK(PN,II),II=1,12)
0089              DO 180 II=1,12
0090      176     IF(XK(PN,II) .LT. 0.)GOTO 181
0091      180     CONTINUE
0092      181     NP(PN)=II-1
0093              XK(PN,II)=0.
0094              GOTO 199
0095      190     IF(IPROC .EQ. 10)GOTO 197
0096              IF(IPROC .EQ. 11)WRITE(INP,195)
0097      195     FORMAT('0PROCESS SPLIT'/' SPLIT?',8)
0098              READ(INP,*)XS(IS1,1)
0099              GOTO 199
0100      197     TYPE *,'PROCESS MIX'
0101      199     CONTINUE
0102      200     WRITE(4'KKK)K,PN,IPROC,IS1,IS2,OS1,OS2,LK
0103              IF(IS1 .EQ. 1)WRITE(IOP,240)
0104      240     FORMAT(1H1,////,55X,'INPUT DATA',///,25X,'K',8X,'PN',
                1 5X,'PROCESS',5X,'IS1',7X,'IS2',7X,'OS1',7X,'OS2',8X,
                2 'LK',//)
0105              IF(K-9 .EQ. 0)GOTO 277
0106              WRITE(IOP,260)K,PN,IPROC,IS1,IS2,OS1,OS2,LK
0107      260     FORMAT(25X,I1,7(8X,I2))
0108      277     KKK=KKK+1
```

```
0109                IF((K-9) .NE. 0)GOTO 120
0110                LLL=0
0111          300   KKK=0
0112                KKK=LLL
0113                K=0
0114                IND=0
0115                IBAD=0
0116                DO 325 I=1,KK
0117                OS1=I
0118          325   CALL PN1
0119          400   KKK=KKK+1
0120                READ(4'KKK)K,PN,IPROC,IS1,IS2,OS1,OS2,LK
0121                IF(PN .EQ. 1)ISF=IS1
0122                IF(PN .NE. 0)IOSF=OS1
0123                IF((LK-9) .EQ. 0)IPN=PN
0124                IF((K-9) .EQ. 0)GOTO 950
0125                IF(IPROC .EQ. 1)CALL SED1
0126                IF(IPROC .EQ. 2)CALL AER2
0127                IF(IPROC .EQ. 3)CALL COX3
0128                IF(IPROC .EQ. 4)CALL COAG4
0129                IF(IPROC .EQ. 5)CALL FIL5
0130                IF(IPROC .EQ. 6)CALL GAC6
0131                IF(IPROC .EQ. 7)CALL THM7
0132                IF(IPROC .EQ. 10)CALL MIX
0133                IF(IPROC .EQ. 11)CALL SPLIT
0134                IF(LK .EQ. 0)GOTO 400
0135                IF(K .EQ. 0)GOTO 400
0136                IF(IND .EQ. 1)GOTO 600
0137                LLL=KKK-1
0138                IND=K
0139                GOTO 400
0140          600   IF((ABS(XM(2,OS1)-TXM(2,OS1)))=(TIT*XM(2,OS1)) .GT. 0.)GOTO 760
0141          650   CONTINUE
0142                IF(OS2 .EQ. 0)GOTO 780
0143          700   IF((ABS(XM(2,OS2)-TXM(2,OS2)))=(TIT*XM(2,OS2)) .GT. 0.)GOTO 760
0144          750   CONTINUE
0145                GOTO 780
0146          760   IBAD=1
0147          780   TXM(2,OS1)=XM(2,OS1)
0148                IF(OS2 .EQ. 0)GOTO 900
0149                TXM(2,OS2)=XM(2,OS2)
0150          900   IF(IBAD .EQ. 1)GOTO 300
0151                IF(K .NE. 2)GOTO 400
0152                LLL=KKK-1
0153                IND=1
0154                GOTO 400
0155          950   WRITE(IOP,970)CHEM
0156                DO 959 I=1,IPN
0157          959   WRITE(IOP,980)(I,(XX(I,J),J=1,NP(I)))
0158          970   FORMAT('0'/42X,'PROCESS RATE CONSTANTS FOR',1X,20A2//25X,'PN'/)
0159          980   FORMAT('0',24X,I2,5(G15.6)/(27X,5(G15.6)))
0160                CALL PRINT
0161         1000   CONTINUE
0162                STOP
0163                END
```

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FORTRAN IV-PLUS V3.0              08:51:23    12-JUN-81          PAGE 1
SED1.FTN;46                /CK/TR:ALL/WR

0001              SUBROUTINE SED1
0002              INTEGER IS1,IS2,OS1,OS2,PN
0003              COMMON /XSM/XS(20,3)
0004              COMMON XM(8,30),TXM(8,30),IP(20),
     1            IS1,IS2,OS1,OS2,XK(20,12),PRS(20),PRC(20),PT(20),PN
0005              DEP=XK(PN,1)
0006              SA=XK(PN,2)
0007              F=XK(PN,3)
0008              IF(SA .NE. 0.)XK(PN,4)=XM(2,IS1)*1000./SA
0009              OF=XK(PN,4)
0010              IF(DEP .NE. 0.)XK(PN,5)=DEP*179.532/OF
0011              DT=XK(PN,5)
0012              FR=.755*EXP(-OF/3247.)
0013              XM(2,OS2)=F*XM(2,IS1)
0014              XM(2,OS1)=XM(2,IS1)-XM(2,OS2)
0015              XM(3,OS2)=FR*XM(2,IS1)*XM(3,IS1)/XM(2,OS2)
0016              XM(3,OS1)=(1.-FR)*XM(2,IS1)*XM(3,IS1)/XM(2,OS1)
0017              QSM=XM(2,OS1)*XM(3,OS1)*XM(4,IS1)+XM(2,OS1)*XM(5,IS1)
0018              QSO=XM(2,IS1)*(XM(3,IS1)*XM(4,IS1)+XM(5,IS1))
0019              XM(5,OS1)=1.
0020              XM(5,OS2)=1.
0021              CALL PN1
0022              PS1=XM(4,OS1)
0023              PS2=XM(4,OS2)
0024              PSO2=(XM(2,OS2)*(1.0+XM(3,OS2)*PS2))
0025              PSO1=(XM(2,OS1)*(1.+XM(3,OS1)*PS1))
0026              XM(5,OS2)=(QSO-QSM)/PSO2
0027              XM(5,OS1)=(QSO-XM(5,OS2)*PSO2)/PSO1
0028              XM(5,OS2)=(QSO-XM(5,OS1)*PSO1)/PSO2
0029              XM(4,OS1)=XM(5,OS1)*PS1
0030              XM(4,OS2)=XM(5,OS2)*PS2
0031              CALL PER
0032              RETURN
0033              END
```

```
FORTRAN IV-PLUS V3.0              08:51:43    12-JUN-81          PAGE 1
AER2.FTN;24                /CK/TR:ALL/WR

0001              SUBROUTINE AER2
0002              INTEGER IS1,IS2,OS1,OS2,PN
0003              COMMON /XSM/XS(20,3)
0004              COMMON XM(8,30),TXM(8,30),IP(20),
     1            IS1,IS2,OS1,OS2,XK(20,12),PRS(20),PRC(20),PT(20),PN
0005              AP=XK(PN,1)
0006              OP=XK(PN,2)
0007              TEMP=XK(PN,3)
0008              TDS=XK(PN,4)
0009              CPD=XK(PN,5)
0010              COX=XK(PN,6)
0011              CV=XK(PN,7)
0012              DT2=XK(PN,8)
0013              CP=XS(1,3)
0014              SMT=XK(PN,9)
0015              XNI=XK(PN,11)
0016              XNW=XK(PN,10)
0017              IF(SMT .EQ. 1.)GOTO 5
0018              OSAT=(4.5-2.67*TDS)*((AP-OP)/(760.-OP))/(33.5+TEMP)
0019              C1=COX*OSAT
0020              C2=(CV+CPD+C1)/(1.+CP*XM(3,IS1)*.000001)
0021              GOTO 10
0022           5  C2=.0608*(44./XNW)**(1/2)
0023              DT2=XNI
0024          10  XM(5,OS1)=XM(5,IS1)*EXP(-C2*DT2)
0025              XM(2,OS1)=XM(2,IS1)
0026              XM(3,OS1)=XM(3,IS1)
0027              XM(4,OS1)=XM(4,IS1)
0028              CALL PER
0029              CALL PN1
0030              RETURN
0031              END
```

```
FORTRAN IV-PLUS V3.0              08:52:02    12-JUN-81          PAGE 1
COX3,FTN;12              /CK/TR:ALL/WR

0001              SUBROUTINE COX3
0002              INTEGER IS1,IS2,OS1,OS2,PN
0003              COMMON XM(8,30),TXM(8,30),IP(20),
          1       IS1,IS2,OS1,OS2,XK(20,12),PRB(20),PRC(20),PT(20),PN
0004              XK2=XK(PN,1)
0005              SLOPE=XK(PN,2)
0006              PH=XK(PN,3)
0007              THETA=XK(PN,4)
0008              CONX=XK(PN,5)
0009              TEMPX=XK(PN,6)
0010              DT3=XK(PN,7)
0011              XM(3,OS1)=XM(3,IS1)
0012              XDX=XK2*EXP(SLOPE*2.303*(PH-7.))*THETA**(TEMPX-20.)*CONX
0013              XM(5,OS1)=XM(5,IS1)*EXP(-XDX*DT3)
0014              XM(2,OS1)=XM(2,IS1)
0015              CALL PN1
0016              CALL PER
0017              RETURN
0018              END
```

```
FORTRAN IV-PLUS V3.0              08:52:16    12-JUN-81          PAGE 1
COAG4,FTN;45             /CK/TR:ALL/WR

0001              SUBROUTINE COAG4
0002              INTEGER IS1,IS2,OS1,OS2,PN
0003              COMMON XM(8,30),TXM(8,30),IP(20),
          1       IS1,IS2,OS1,OS2,XK(20,12),PRB(20),PRC(20),PT(20),PN
0004              IF(XK(PN,4) .EQ. 1)GOTO 5
0005              GTF=-.052-(.07774*XK(PN,1)**.305)
0006              XKPN=(GTF*XK(PN,2)*2.303)
0007              GOTO 10
0008         5    XKPN=.891*XM(2,IS1)*XK(PN,5)
0009        10    XM(2,OS1)=XM(2,IS1)*(1.-XK(PN,3))
0010              XM(2,OS2)=XM(2,IS1)*XK(PN,3)
0011              XM(3,OS1)=XM(3,IS1)*EXP(XKPN)
0012              QST=XM(2,IS1)*XM(3,IS1)-XM(2,OS1)*XM(3,OS1)
0013              XM(3,OS2)=QST/XM(2,OS2)
0014              QSN=XM(2,OS1)*XM(3,OS1)*XM(4,IS1)+XM(2,OS1)*XM(5,IS1)
0015              QSO=XM(2,IS1)*(XM(3,IS1)*XM(4,IS1)+XM(5,IS1))
0016              XM(5,OS1)=1.
0017              XM(5,OS2)=1.
0018              CALL PN1
0019              PS1=XM(4,OS1)
0020              PS2=XM(4,OS2)
0021              PS02=(XM(2,OS2)*(1.0+XM(3,OS2)*PS2))
0022              PS01=(XM(2,OS1)*(1.+XM(3,OS1)*PS1))
0023              XM(5,OS2)=(QSO-QSN)/PS02
0024              XM(5,OS1)=(QSO-XM(5,OS2)*PS02)/PS01
0025              XM(5,OS2)=(QSO-XM(5,OS1)*PS01)/PS02
0026              XM(4,OS1)=XM(5,OS1)*PS1
0027              XM(4,OS2)=XM(5,OS2)*PS2
0028              CALL PER
0029              RETURN
0030              END
```

```
FORTRAN IV-PLUS V3.0              08:52:36    12-JUN-81          PAGE 1
FIL5,FTN;25              /CK/TR:ALL/WR

0001              SUBROUTINE FIL5
0002              INTEGER IS1,IS2,OS1,OS2,PN
0003              COMMON XM(8,30),TXM(8,30),IP(20),
          1       IS1,IS2,OS1,OS2,XK(20,12),PRB(20),PRC(20),PT(20),PN
0004              XM(5,OS1)=XM(5,IS1)
0005              XM(5,OS2)=XM(5,IS1)
0006              XKPF=(XK(PN,2)-(XK(PN,3)*XK(PN,1)/XM(2,IS1)))
0007              XM(3,OS1)=XM(3,IS1)**XK(PN,4)*EXP(XKPF)
0008              XM(2,OS1)=XM(2,IS1)*.96
0009              XM(2,OS2)=XM(2,IS1)-XM(2,OS1)
0010              XM(3,OS2)=(XM(2,IS1)*XM(3,IS1)-XM(2,OS1)*XM(3,OS1))/
          1       (XM(2,OS2))
0011              CALL PN1
0012              CALL PER
0013              RETURN
0014              END
```

```
0001            SUBROUTINE GAC6
0002            COMMON /XSM/XS(20,3)
0003            COMMON /IO/IOP,INP
0004            COMMON XM(8,30),TXM(8,30),IP(20),
               1 IS1,IS2,OS1,OS2,XK(20,12),PRS(20),PRC(20),PT(20),PN
0005            INTEGER IS1,IS2,OS1,OS2,PN
0006            REAL NSC,KFC,KFA,KA,KFB,NCPC,NRE,MAXD
0007            DATA DCP,GAMMA,EPS,DENBIO,DENCP,Y,SINT,SMAX,DENW,
               1 G,DENPAC,ACID,NSC/.001,3.61E-3,0.45,1.0E+6,1.35E+06,
               2 0.67,2.5,265.,0.998E6,9.5E+04,400417.,67.E-06,1425.928/
0008            DATA XAV/187.42/
C               DCP    = DIAMETER OF CARBON PARTICLE
C               GAMMA  = KINEMATIC VISCOSITY OF WATER
C               EPS    = PACKED CARBON BED POROSITY
C               DENBIO = DENSITY OF BIOMASS
C               DENCP  = DENSITY OF CARBON PARTICLE
C               Y      = YIELD COEFFICIENT FOR BIOMASS GROWTH
C               SINT   = INTERNAL BIOMASS SUBSTRATE CONC
C               SMAX   = SUBSTRATE CONC AT WHICH MASS TRANSFER NO LONGER LIMITS
C               DENW   = DENSITY OF WATER
C               G      = GRAVITATIONAL CONSTANT
C               DENPAC = PACKED BED DENSITY OF CARBON
C               ACID   = MAXIMUM ACTIVE THICKNESS OF BICFILM
C               NSC    = SCHMIDT NUMBER
C               VOLCAR = VOLUME CARBON OCCUPIER PER CSTR
C               NCPC   = NUMBER OF CARBON PARTICLES PER CSTR
C               VOLACT = VOLUME OF ACTIVE BIOMASS PER CSTR
C               AREA   = CROSS-SECTIONAL AREA OF CONTACTOR
C               CARBON = VOLUME OF CARBON PER  CSTR
C               DL     = DIFFUSIVITY OF CHEMICAL IN WATER
0009            AREA=XK(PN,2)
0010            CARBON=XK(PN,3)
0011            DL=XK(PN,4)
0012            XM(2,OS1)=XM(2,IS1)
0013            XM(4,IS1)=CP*DENCP*XM(5,IS1)/
               1 (DENW*1000000.+DENCP-XM(3,IS1))
0014            IF(XK(PN,1) .EQ. 0.)XK(PN,1)=1.0E-06
0015            VOLCAR = 1000.*(88./21.)*((.5*DCP)**3)
0016            NCPC = DENPAC*CARBON/(DENCP*VOLCAR*(1.-EPS))
0017            VOLACT=(1000.*(88./21.)*((.5*DCP+ACTD)**3)-VOLCAR
0018            VSA = 157.708*XM(2,IS1)/AREA
0019            NRE = (DCP+2.*XK(PN,1))*VSA/GAMMA
0020            MAXD = (0.68*EXP(12.17/NRE))*1.E-06
0021            VOLBIO = (1000.*(88./21.)*((.5*DCP+XK(PN,1)))**3-VOLCAR
0022            DENBC = (VOLCAR*DENCP+VOLBIO*DENBIO)/(VOLCAR+VOLBIO)
0023            EPSI = ((13.86*(DENW**0.4)*((DENW*GAMMA)**0.6)*(VSA**1.4))/
               1 (((DCP+2.*XK(PN,1))**1.6)*G*(DENBC-DENW)))**0.18
0024            PE = (1.-EPS)/(1.-EPSI)
0025            IF(PE .LT. 1.1) WRITE(INP,20) PE
0026         20 FORMAT(3X,'CAUTION ADSORBER IS UNDER-EXPANDED ',F5.2)
0027         31 XK(PN,1)=((21./88000.)*(VOLCAR+(XAV*
               1 PE*CARBON)/(NCPC*DENBIO)))**(1./3.)-.5*DCP
0028            IF(XK(PN,1) .GT. MAXD) SLUF=1.0
0029            IF(XK(PN,1) .LE. MAXD) SLUF=0.0
0030            IF(XK(PN,1) .GT. MAXD) XK(PN,1)=MAXD
0031            IF(XK(PN,1) .GT. ACTD) XAV=NCPC*
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FORTRAN IV-PLUS V3.0              08:52:49    12-JUN-81          PAGE 2
GAC6.FTN;24                /CK/TR:ALL/WR

     1 VOLACT*DENBIO/(PE*CARBON)
0032      34 KFC = (1.34*(NRE/(1.-EPSI))**(-.468))*VSA/NSC**(2./3.)
0033         IF(XK(PN,1) .GT. 0.0) KFB = BSADL/XK(PN,1)
0034         IF(XK(PN,1) .GT. 0.0) KF=1./((1./KFC)+(1./KFB))
0035         IF(XK(PN,1) .LE. 0.0) KF=KFC
0036         KFA = KF*(1000*(NCPC*(88./7.)*(.5*DCP+XK(PN,1))**2)/(PE*CARBON))
0037         BSTAR = 10.**((XM(4,IS1/1000.)+.0711)/.1552)
0038         THETX = (EPSI*PE*CARBON)/XM(2,IS1)
0039         KB = KFC*88.*NCPC*(.5*DCP+XK(PN,1))**2/(100.*PE*CARBON)
0040         IF(XM(5,IS1) .LE. SINT) RXS=0.0
0041         IF(XM(5,IS1) .LE. SMAX .AND. XM(5,IS1)
     1    .GT. SINT) RXS=KB*(XM(5,IS1)-SINT)
0042         IF(XM(5,IS1) .GT. SMAX) RXS=KB*(SMAX-SINT)
0043         IXM(5,OS1) = 0.0
0044         RXC = KFA*(XM(5,IS1)-BSTAR)
0045         XM(3,OS1)=XM(3,IS1)+THETX*SLUF*Y*RXS
0046      41 XM(5,OS1)=XM(5,IS1)-THETX*(RXC+RXS)
0047         IF((ABS(XM(5,OS1)-IXM(5,OS1)))=(0.05*XM(5,OS1)) .LE. 0.) GO TO 42
0048         IXM(5,OS1)=XM(5,OS1)
0049         RXC = KFA*(XM(5,OS1)-BSTAR)
0050         GO TO 41
0051      42 XM(4,OS1) = CP*RHOCP*XM(5,OS1)/
     1    (DENW*1000000.*RHOCP-XM(3,OS1))
0052         CALL PER
0053         RETURN
0054         END
```

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FORTRAN IV-PLUS V3.0              08:53:15    12-JUN-81          PAGE 1
THM7.FTN;5                 /CK/TR:ALL/WR

0001              SUBROUTINE THM7
0002              INTEGER IS1,IS2,OS1,OS2,PN
0003              COMMON XM(8,30),IXM(8,30),IP(20),
     1         IS1,IS2,OS1,OS2,XK(20,12),PRS(20),PRC(20),PT(20),PN
0004              DO 1 I=2,3
0005         1    XM(I,OS1)=XM(I,IS1)
0006              XM(5,OS1)=XM(5,IS1)*EXP(XK(PN,1))
0007              CALL PN1
0008              CALL PER
0009              RETURN
0010              END
```

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FORTRAN IV-PLUS V3.0              08:54:02    12-JUN-81          PAGE 1
MIX.FTN;6                  /CK/TR:ALL/WR

0001              SUBROUTINE MIX
0002              INTEGER IS1,IS2,OS1,OS2,PN
0003              COMMON XM(8,30),IXM(8,30),IP(20),
     1         IS1,IS2,OS1,OS2,XK(20,12),PRS(20),PRC(20),PT(20),PN
0004              XM(2,OS1)=XM(2,IS1)+XM(2,IS2)
0005              IF(XM(2,OS1) .EQ. 0.)RETURN
0006              TXM1=XM(2,IS1)/(XM(2,IS1)+XM(2,IS2))
0007              IXM2=XM(2,IS2)/(XM(2,IS1)+XM(2,IS2))
0008              DO 10 I=3,8
0009         10   XM(I,OS1)=IXM1*XM(I,IS1)+IXM2*XM(I,IS2)
0010              RETURN
0011              END
```

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FORTRAN IV-PLUS V3.0              08:54:15    12-JUN-81          PAGE 1
SPLIT.FTN;13              /CK/TR:ALL/WR

0001                SUBROUTINE SPLIT
0002                INTEGER IS1,IS2,OS1,OS2,PN
0003                COMMON /XSM/XS(20,3)
0004                COMMON XM(8,30),TXM(8,30),IP(20),
               1    IS1,IS2,OS1,OS2,XK(20,12),PRS(20),PRC(20),PT(20),PN
0005                XM(2,OS2)=XS(IS1,1)*XM(2,IS1)
0006                IF(XS(IS1,1) .EQ. 0.)XM(2,OS2)=.5*XM(2,IS1)
0007                XM(2,OS1)=XM(2,IS1)-XM(2,OS2)
0008                DO 10 I=3,8
0009                XM(I,OS1)=XM(I,IS1)
0010          10    XM(I,OS2)=XM(I,IS1)
0011                RETURN
0012                END
```

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FORTRAN IV-PLUS V3.0              08:53:32    12-JUN-81          PAGE 1
PN1.FTN;30                /CK/TR:ALL/WR

0001                SUBROUTINE PN1
0002                INTEGER IS1,IS2,OS1,OS2,PN
0003                COMMON /XSM/XS(20,3)
0004                COMMON XM(8,30),TXM(8,30),IP(20),
               1    IS1,IS2,OS1,OS2,XK(20,12),PRS(20),PRC(20),PT(20),PN
0005                DENW=XS(1,1)
0006                DENS=XS(1,2)
0007                IF(DENW .EQ. 0.)DENW=1.
0008                IF(DENS .EQ. 0.)DENS=1.2
0009                CP=XS(1,3)
0010                XM(4,OS1)=CP*DENS*XM(5,OS1)/(DENW*(1000000.*DENS+
               1    XM(3,OS1)))
0011                IF(OS2 .EQ. 0)RETURN
0012                XM(4,OS2)=CP*DENS*XM(5,OS2)/(DENW*(1000000.*DENS+
               1    XM(3,OS2)))
0013                RETURN
0014                END
```

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FORTRAN IV-PLUS V3.0              08:53:48    12-JUN-81          PAGE 1
PER.FTN;17                /CK/TR:ALL/WR

0001                SUBROUTINE PER
0002                INTEGER IS1,IS2,OS1,OS2,PN
0003                COMMON XM(8,30),TXM(8,30),IP(20),
               1    IS1,IS2,OS1,OS2,XK(20,12),PRS(20),PRC(20),PT(20),PN
0004                A=((XM(2,IS1)*XM(3,IS1)*XM(4,IS1))-(XM(2,OS1)*XM(3,OS1)
               1    *XM(4,OS1)))
0005                B=XM(3,IS1)*XM(4,IS1)*XM(2,IS1)+XM(2,IS1)*XM(5,IS1)
0006                C=(XM(2,IS1)*XM(5,IS1)-XM(5,OS1)*XM(2,OS1))
0007                PRS(PN)=A/B*100.
0008                PRC(PN)=C/B*100.
0009                PT(PN)=(A+C)/B*100.
0010                RETURN
0011                END
```

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FORTRAN IV-PLUS V3.0            08:50:56    12-JUN-81          PAGE 1
PRINT,FTN;66                /CK/TR:ALL/WR

0001                SUBROUTINE PRINT
0002                INTEGER IS1,IS2,OS1,OS2,PN
0003                COMMON /XSM/XS(20,3)
0004                COMMON /C/CHEM(20)
0005                COMMON /IO/IOP,INP
0006                COMMON /IFP/ISF,IOSF
0007                COMMON XM(8,30),IXM(8,30),IP(20),
          1     IS1,IS2,OS1,OS2,XK(20,12),PRS(20),PRC(20),PT(20),PN
0008                WRITE(IOP,1)CHEM
0009         1      FORMAT(1H1//55X,'STREAM CHARACTERISTICS'//65X,'VOLUME FLOW,
                1  MILLIONS OF GALLONS PER DAY'/65X,'SEDIMENT, MILLIGRAMS',1X,
                2  'PER LITRE'/65X,20A2/66X,'CONCENTRATION ON SEDIMENT, MILLIGRAMS',1X,
                3  'PER GRAM'/66X,'CONCENTRATION, MICROGRAMS PER LITRE'/)
0010                DO 20 I=1,16
0011                IF(XM(1,I) .EQ. 0.)GOTO 20
0012                WRITE(IOP,102)
0013                WRITE(IOP,103)(XM(J,I),J=1,5)
0014          20    CONTINUE
0015         102    FORMAT(5X,'STREAM',12X,'Q',9X,'SED',8X,'XM',9X,'CON')
0016         103    FORMAT(7X,F3.0,6X,2(F11.3),E11.4,F11.4//)
0017                WRITE(IOP,104)
0018         104    FORMAT(1H1//45X,'PROCESS CHARACTERISTICS'////)
0019                DO 1000 I=1,16
0020                IF(IP(I) .GE. 10)GOTO 1000
0021                IF(IP(I) .EQ. 0)GOTO 1100
0022
0023                KK=IP(I)
0024                GOTO(110,120,130,140,150,160,170),KK
0025         110    WRITE(IOP,111)I,PRS(I),PRC(I),PT(I),XK(I,2),XS(1,3),XK(I,4),
                1  XK(I,5)
0026         111    FORMAT(2X,1HP,I2,'PLAIN',14X,'PERCENT REMOVAL',13X,'SA',
                1  9X,'CP',9X,'OF',9X,'DT'/5X,'SEDIMENTATION',2X,'SED',6X,'WATER',
                2  5X,'TOTAL'/18X,3(G10.3),4(G11.4)//)
0027                GOTO 1000
0028         120    WRITE(IOP,121)I,PRS(I),PRC(I),PT(I),(XK(I,L),L=5,8)
0029         121    FORMAT(2X,1HP,I2,'AERATION',11X,'PERCENT REMOVAL',12X,'KPD',8X,
                1  'KOX',8X,'KV',10X,'DT'/20X,'SED',6X,'WATER',5X,'TOTAL'/18X,
                2  3(G10.3),4(G11.4)//)
0030                GOTO 1000
0031         130    WRITE(IOP,131)I,PRS(I),PRC(I),PT(I),(XK(I,L),L=1,7,2)
0032         131    FORMAT(2X,1HP,I2,'CHEMICAL',11X,'PERCENT REMOVAL',13X,'K2',9X,
                1  'PH',8X,'COX',9X,'DT'/5X,'OXIDATION',8X,'SED',6X,'WATER',5X,
                2  'TOTAL'/18X,3(G10.3),4(G11.4)//)
0033                GOTO 1000
0034         140    WRITE(IOP,141)I,PRS(I),PRC(I),PT(I),(XK(I,L),L=1,3)
0035         141    FORMAT(2X,1HP,I2,'COAGULATION-',7X,'PERCENT REMOVAL',13X,'TF',9X,
                1  'TS',9X,'FUF'/5X,'FLOCCULATION',3X,'SED',6X,'WATER',5X,
                2  'TOTAL'/18X,3(G10.3),3(G11.4)//)
0036                GOTO 1000
0037         150    WRITE(IOP,151)I,PRS(I),PRC(I),PT(I),(XK(I,L),L=1,4)
0038         151    FORMAT(2X,1HP,I2,'FILTRATION',9X,'PERCENT REMOVAL',13X,'SA',9X,
                1  'K1',9X,'K2',9X,'K3'/20X,'SED',6X,'WATER',5X,
                2  'TOTAL'/18X,3(G10.3),4(G11.4)//)
0039                GOTO 1000
0040         160    WRITE(IOP,161)I,PRS(I),PRC(I),PT(I),(XK(I,L),L=1,4)
0041         161    FORMAT(2X,1HP,I2,'CARBON',13X,'PERCENT REMOVAL',13X,'K1',9X,
                1  'K2',9X,'K3',9X,'DT'/5X,'ADSORPTION',5X,'SED',6X,'WATER',5X,
                2  'TOTAL'/18X,3(G10.3),4(G11.4)//)
0042                GOTO 1000
0043         170    WRITE(IOP,171)I,PRS(I),PRC(I),PT(I),(XK(I,L),L=1,4)
0044         171    FORMAT(2X,1HP,I2,'CHLORINATION',7X,'PERCENT REMOVAL',13X,
                1  'K1',9X,'K2',9X,'K3',9X,'DT'/20X,'SED',6X,'WATER',5X,
                2  'TOTAL'/18X,3(G10.3),4(G11.4)//)
0045        1000    CONTINUE
0046        1100    A=((XM(2,ISF)*XM(3,ISF)*XM(4,ISF))-(XM(2,IOSF)*XM(3,IOSF)
                1  *XM(4,IOSF)))
0047                B=XM(3,ISF)*XM(4,ISF)*XM(2,ISF)+XM(2,ISF)*XM(5,ISF)
0048                C=(XM(2,ISF)*XM(5,ISF)-XM(5,IOSF)*XM(2,IOSF))
0049                FPRS=A/B*100.
0050                FPRC=C/B*100.
0051                FPT=(A+C)/B*100.
0052                WRITE(IOP,1111)CHEM,FPRS,FPRC,FPT
0053        1111    FORMAT(1X,20A2/1X,'PERCENT REMOVAL WITH SEDIMENT=',G11.4/1X,
                1  'PERCENT REMOVAL IN THE AQUEOUS PHASE=',G11.4/1X,'TOTAL REMOVAL
                2  =',G11.4,'PERCENT')
0054                RETURN
0055                END
```